Self-similar Gaussian processes for modeling anomalous diffusion

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(Received 8 April 2002; published 29 August 2002)

We study some Gaussian models for anomalous diffusion, which include the time-rescaled Brownian motion, two types of fractional Brownian motion, and models associated with fractional Brownian motion based on the generalized Langevin equation. Gaussian processes associated with these models satisfy the anomalous diffusion relation which requires the mean-square displacement to vary with t^{α}, $0<\alpha<2$. However, these processes have different properties, thus indicating that the anomalous diffusion relation with a single parameter is insufficient to characterize the underlying mechanism. Although the two versions of fractional Brownian motion and time-rescaled Brownian motion all have the same probability distribution function, the Slepian theorem can be used to compare their first passage time distributions, which are different. Finally, in order to model anomalous diffusion with a variable exponent $\alpha(t)$ it is necessary to consider the multifractional extensions of these Gaussian processes.

DOI: 10.1103/PhysRevE.66.021114 PACS number(s): 05.40.−a, 02.50.Ey

I. INTRODUCTION

Anomalous diffusion occurs in many physical and biological systems [1–3]. It is characterized by the following mean-square displacement (for the one-dimensional case):

$$\langle x^2(t)\rangle \sim t^{\alpha}, \quad 0<\alpha<2. \tag{1}$$

For $0<\alpha<1$, $x(t)$ represents subdiffusion (or suppressed diffusion), and for $1<\alpha<2$ it is called superdiffusion (or enhanced diffusion), while $\alpha=1$ corresponds to the normal diffusion or Brownian motion.

There have been many attempts to model anomalous diffusion by means of generalized diffusion equations, which mostly provide a mathematical description of the process, in particular, the second moments of the solutions of these equations are shown to exhibit the desired time dependence (1). Despite the various models proposed for anomalous diffusion (see, for example, [2,4]), there still exists a need to obtain a deeper understanding of its underlying mechanism.

In this paper, we study some Gaussian models of anomalous diffusion. Even though all these Gaussian processes satisfy the anomalous diffusion relation (1), they have quite different properties. We then consider the Langevin equation approach with a solution that can be linked to fractional Brownian motion either asymptotically or in the high frequency limit. An explanation and solution are given for the anomaly that exists in the generalized Langevin equation approach, which gives asymptotic mean-square displacement for $\alpha=1$ as $t\ln t$ instead of t as required for Brownian motion. Two types of fractional Langevin equations and their suitability for modeling anomalous diffusion are considered. We next show that the Slepian theorem can be used to compare the first passage time distributions of the three Gaussian processes, namely, the two versions of fractional Brownian motion and the time-rescaled Brownian motion. Finally, we generalize the fractional Brownian motion, fractional Ornstein-Uhlenbeck process, and the time-rescaled Brownian motion to their corresponding "multifractional" processes. Their local properties are studied to see whether they can be used to model anomalous diffusion with variable scaling exponents.

II. TIME-RESCALED BROWNIAN MOTION

The simplest Gaussian model that satisfies the anomalous diffusion relation (1) can be derived by time rescaling the Brownian motion $X(t)$ using the following nonlinear time transformation:

$$t \rightarrow t_* = t^{\alpha}, \quad 0<\alpha<2, \tag{2}$$

to obtain the time-rescaled Brownian motion [or scaled Brownian motion (SBM)] $X_*(t) \equiv X(t_*)$, which is again a Gaussian process with mean zero and correlation function

$$\langle X(t_*)X(s_*)\rangle = t_* \wedge s_* = t^{\alpha}\wedge s^{\alpha} = \langle X_*(t)X_*(s)\rangle, \tag{3}$$

where $\wedge$ denotes the minimum. Note that $X_*(t)$ can also be defined in terms of white noise $\eta(t)$:

$$X_*(t) = \int_0^t u^{\alpha-1/2}\eta(u)\,du, \tag{4}$$

where $\eta(t)$ satisfies $\langle \eta(t)\eta(s)\rangle = \delta(t-s)$. The differential version of Eq. (4) is

$$\frac{dX_*(t)}{dt} = t^{(\alpha-1)/2}\eta(t). \tag{5}$$

It can be easily verified that the variance of $X_*(t)$ satisfies (1).

The SBM $X_*(t)$ preserves the basic properties of Brownian motion. Just like Brownian motion, $X_*(t)$ is a Gaussian Markov process since for $t>0$, the scaling transformation $t \rightarrow t^{\alpha}$, $\alpha>0$ preserves the time ordering, hence the Markov property. One can also prove the Markov property for SBM by verifying the Chapman-Kolmogorov equation using its

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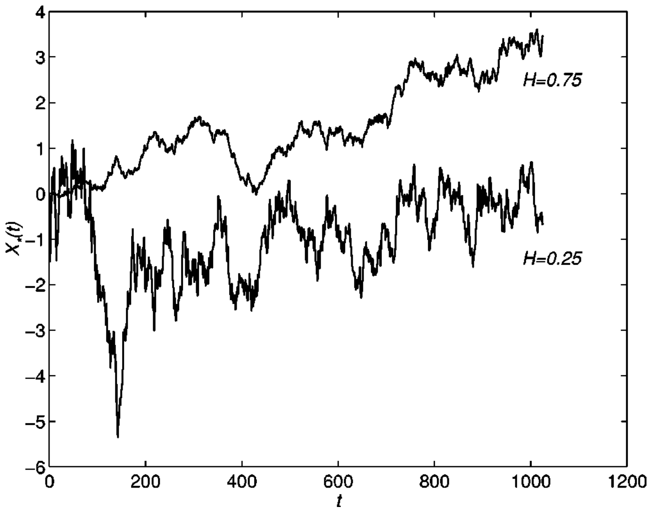

FIG. 1. The sample paths of rescaled Brownian motion with $H=0.25$ and $H=0.75$.

probability distribution function. $X_*(t)$ is a self-similar process with scaling exponent $\alpha/2$. For $b>0$, we have

$$\langle X_*(bt)X_*(bs)\rangle = \langle X([bt]^\alpha)X([bs]^\alpha)\rangle = b^\alpha \langle X_*(t)X_*(s)\rangle, \tag{6}$$

where we have used the self-similar property of Brownian motion, $X(bt)=b^{1/2}X(t)$. Similarly, one can verify that the SBM has independent increments for nonoverlapping intervals, just like in the case of ordinary Brownian motion. The sample paths of the rescaled Brownian motions simulated using the time-rescaling transformation of Brownian motion are shown in Fig. 1. For $H=0.75$, $X_*(t)$ represents an accelerated Brownian motion; and for $H=0.25$ it becomes decelerated Brownian motion. (Refer to Appendix A for the details of numerical algorithms.)

Brownian motion $X(t)$ satisfies the diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}, \tag{7}$$

with $P(x,t)$ the probability distribution function (PDF) for the Brownian motion, and D the diffusion constant. When subjected to initial condition $P(x,0)=\delta(x)$, Eq. (7) has the solution

$$P(x,t) = \frac{1}{\sqrt{4D\pi t}}\exp\left[-\frac{x^2}{4Dt}\right]. \tag{8}$$

The diffusion equation for the SBM has the same form as Eq. (7), that is,

$$\frac{\partial P(x,t_*)}{\partial t_*} = D\frac{\partial^2 P(x,t_*)}{\partial x^2}, \tag{9}$$

and with initial condition $P(x,t_*=0)=\delta(x)$, its solution is

$$P(x,t_*) = \frac{1}{\sqrt{4D\pi t_*}}\exp\left[-\frac{x^2}{4Dt_*}\right] = \frac{1}{\sqrt{4D\pi t^\alpha}}\exp\left[-\frac{x^2}{4Dt^\alpha}\right] \equiv P_*(x,t). \tag{10}$$

By using

$$\frac{d}{dt} = \frac{dt_*}{dt}\frac{d}{dt_*} = \alpha t^{\alpha-1}\frac{d}{dt_*}, \tag{11}$$

Eq. (9) can be written as

$$\frac{\partial P_*(x,t)}{\partial t} = \alpha D t^{\alpha-1}\frac{\partial^2 P_*(x,t)}{\partial x^2} = D_*(t)\frac{\partial^2 P_*(x,t)}{\partial x^2}, \tag{12}$$

where $D_*(t)=\alpha D t^{\alpha-1}$ can be regarded as the time-dependent diffusion coefficient. Equation (12) is also known as the effective Fokker-Planck equation, which has solution (10) when subjected to initial condition $P_*(x,0)=\delta(x)$.

The PDF given in Eq. (10) is self-similar under the scaling transformations $t\to bt$ and $x\to b^{\alpha/2}x$, thus one gets

$$P_*(b^{\alpha/2}x,bt) = b^{\alpha/2}P_*(x,t). \tag{13}$$

We shall show below that fractional Brownian motion also has the same PDF.

III. FRACTIONAL BROWNIAN MOTION

Fractional Brownian motion (FBM) can be regarded as a natural generalization of Brownian motion from the perspective of the Langevin equation. Recall that the following Langevin equation:

$$\frac{dX(t)}{dt} = F(X(t),t) + \eta(t) \tag{14}$$

has Brownian motion as the solution in the absence of external force $[F(X,t)=0]$:

$$X(t) = \int_0^t \eta(\tau)d\tau. \tag{15}$$

Now one considers the fractional Langevin equation for a free particle,

$$\frac{d^\beta X(t)}{dt^\beta} = \eta(t), \tag{16}$$

where the fractional derivative can be defined in terms of the fractional integral ${}_aI_t^\beta$ [5],

$${}_aI_t^\beta f(t) = \frac{1}{\Gamma(\beta)}\int_a^t (t-u)^{\beta-1}f(u)du \quad \text{for} \quad \beta>0. \tag{17}$$

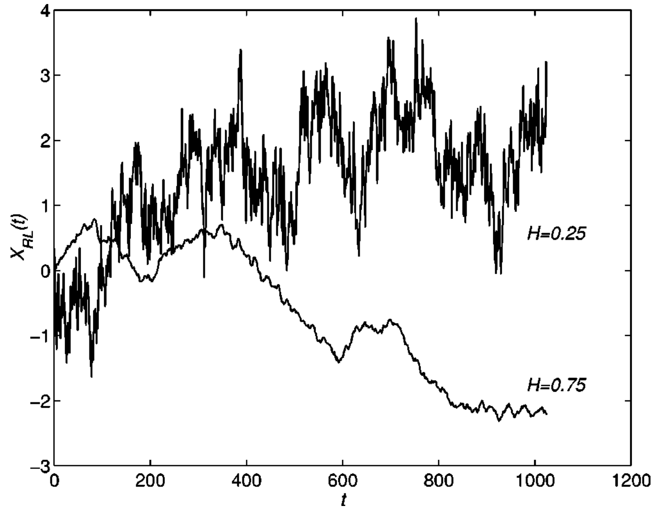

FIG. 2. The sample paths of RL-FBM for $H=0.25$ and $H=0.75$.

For $\gamma=-\beta>0$, the fractional derivative ${}_aD_t^\gamma$ is then defined as a fractional integral of order $n-\gamma$ (with $n-1<\gamma<n$) and an ordinary derivative of order n:

$$ {}_aD_t^\gamma f(t)=\left(\frac{d}{dt}\right)^n {}_aD_t^{\gamma-n} f(t). \tag{18}$$

For $a=0$, Eqs. (17) and (18) are known, respectively, as the fractional integral and the fractional derivative of the Riemann-Liouville type; when $a=-\infty$, they are known as the Weyl fractional integral and derivative.

Let the fractional derivative in Eq. (16) be of the Riemann-Liouville type. Inverting Eq. (16) results in

$$X_{\mathrm{RL}}(t)={}_0I_t^\beta \eta(t)=\frac{1}{\Gamma(\beta)}\int_0^t (t-u)^{\beta-1}\eta(u)du, \tag{19}$$

which is known as the fractional Brownian motion of the Riemann-Liouville type (RL-FBM) [6]. Here, we follow the standard notational convention of the fractional calculus with index β, instead of using the Hurst exponent H $(=\beta+1/2)$, $0<H<1$ commonly adopted to index FBM. Note that X_{RL} is well defined for $H>-1/2$. However, for the purpose of comparison with the standard FBM which is defined for $0<H<1$, we shall confine X_{RL} to the same range of H. The sample paths of RL-FBM are shown in Fig. 2 simulated using the algorithms described in Appendix A. $X_{\mathrm{RL}}(t)$ is a self-similar Gaussian process with zero mean and a rather complicated correlation function:

$$\langle X_{\mathrm{RL}}(t)X_{\mathrm{RL}}(s)\rangle=\frac{t^{\beta-1}s^\beta}{\beta[\Gamma(\beta)]^2}\,{}_2F_1\left(1-\beta,1,1+\beta,\frac{s}{t}\right) \tag{20}$$

for $s<t$, and ${}_2F_1$ is the Gauss hypergeometric function. However, the variance of X_{RL} has the following simple form:

$$\langle X_{\mathrm{RL}}^2(t)\rangle=\frac{t^{2\beta-1}}{(2\beta-1)[\Gamma(\beta)]^2}=C_\beta t^{2\beta-1}, \tag{21}$$

which satisfies the anomalous diffusion relation (1) for $\beta=(\alpha+1)/2$ with $\frac{1}{2}<\beta<\frac{3}{2}$. For a Gaussian process, the PDF is completely determined from the knowledge of its variance and mean (here assumed to be zero). Therefore the PDF of RL-FBM is similar to that for SBM:

$$P_{\mathrm{RL}}(x,t)=\frac{1}{\sqrt{4C_\beta \pi t^{2\beta-1}}}\exp\left[-\frac{x^2}{4C_\beta t^{2\beta-1}}\right]. \tag{22}$$

$P_{\mathrm{RL}}(x,t)$ will be equal to $P_*(x,t)$ if the RL-FBM is taken as $D\sqrt{C_\beta}X_{\mathrm{RL}}(t)$. In contrast to $X_*(t)$, $X_{\mathrm{RL}}(t)$ does not satisfy the Markov property. In fact, the presence of time convolution in Eq. (19) is a typical manifestation of long-range memory. There exists a suggestion that the effective Fokker-Planck equation (12) is the diffusion equation for FBM, and the non-Markovian feature is expressed through a time-dependent diffusion constant $D_*=\alpha Dt^{\alpha-1}$ [7]. This statement is invalid since the diffusion equation (12) which is linear in time derivative also describes the Markovian SBM. The non-Markovian character of FBM implies that Eq. (12) does not fully describe FBM, notably it does not allow one to derive its covariance. This remark is further reinforced in our discussion on first passage time distributions of these processes later on.

We note that the RL-FBM is not the standard FBM that is used widely in modeling Gaussian self-similar processes. The standard FBM X_{W} is defined in terms of a modified or reduced fractional integral of the Weyl type [8]:

$$X_{\mathrm{W}}(t)=\frac{1}{\Gamma(\beta)}\left[\int_{-\infty}^t (t-u)^{\beta-1}\eta(u)du - \int_{-\infty}^0 (-u)^{\beta-1}\eta(u)du\right] \tag{22$'$}$$

$$=X_{\mathrm{RL}}\;\frac{1}{\Gamma(\beta)}\int_{-\infty}^0[(t-u)^{\beta-1}-(-u)^{\beta-1}]\eta(u)du. \tag{22$''$}$$

FBM defined by the Weyl fractional integral alone [i.e., the first term of Eq. (22′)] is divergent, hence it is necessary to introduce a compensation term to ensure the convergence. One can regard the standard FBM X_{W} as the sum of two independent Gaussian process: X_{RL} and a process that represents *a history of infinite past* as in Eq. (24″). In other words, X_{W} has a *head start* over X_{RL}, which begins at time $t=0$ with no memory of the past. As a result, the increments of X_{W} satisfy the stationary property, whereas they fail to be so for X_{RL}. In fact, the standard FBM is the only Gaussian self-similar process with stationary increments. Its correlation function has the following simple form:

$$\langle X_{\mathrm{W}}(t)X_{\mathrm{W}}(s)\rangle=\frac{V_H}{2}[|t|^{2H}+|s|^{2H}-|t-s|^{2H}], \tag{23}$$

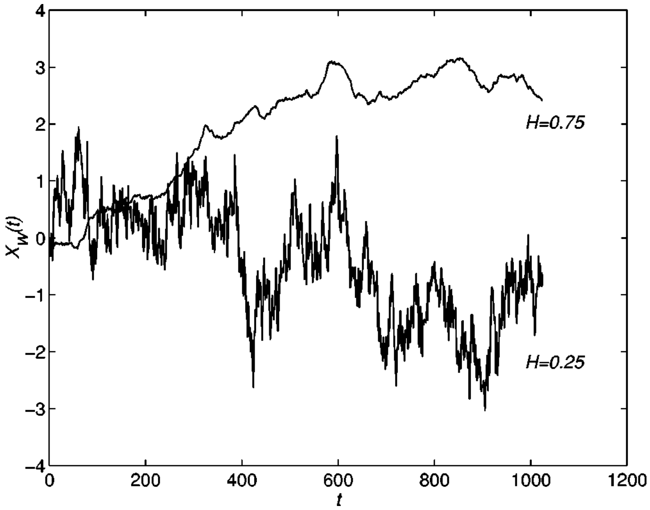

FIG. 3. The sample paths of the standard FBM for $H=0.25$ and $H=0.75$.

where $V_H=[\Gamma(1-2H)\cos(H\pi)]/H\pi$ and $0<H<1$.

In order to obtain a differential version of Eq. (22′) one rewrites $X_W(t)$ as

$$X_W(t)=I_W^\beta\eta(t)-I_W^\beta\eta(0), \tag{24}$$

where I_W^β denotes the Weyl fractional integral of order β. Due to the additional term $I_W^\beta\eta(0)$, one cannot directly apply the inverse operation to obtain a stochastic differential equation similar to Eq. (16) for X_{RL}. However, from Eq. (22′) one gets

$$\frac{dX_W(t)}{dt}=\frac{d}{dt}I_W^\beta\eta(t)=I_W^\gamma\eta(t), \tag{25}$$

with $\gamma=\beta-1$. For $\gamma<0$, Eq. (25) can be written as

$$\frac{dX_W(t)}{dt}=\mathcal{D}_W^{-\gamma}\eta(t), \tag{26}$$

where $\mathcal{D}_W^{-\gamma}$ is the Marchaud fractional derivative [5] defined for sufficiently good $f(t)$ by

$$\mathcal{D}_W^\alpha f(t)=\frac{\alpha}{\Gamma(1-\alpha)}\int_{-\infty}^t\frac{f(t)-f(u)}{(t-u)^{1+\alpha}}du. \tag{27}$$

In other words, $X_W(t)$ does not satisfy a fractional stochastic differential equation of a simple form as in the case of $X_{RL}(t)$ [to be more exact Eq. (25) is a fractional integro-differential equation]. In order to see the link between RL-FBM and the standard FBM, we first note that for $t/\tau\gg1$, the increment $X_{RL}(t+\tau)-X_{RL}(t)$ is stationary. Furthermore, it can be shown that in the large-time asymptotic limit, RL-FBM approaches the standard FBM in the following sense [9]: X_{RL} has stationary increments as $t\to\infty$, with the increment process of X_{RL} approaching increment process of X_W in the mean-square limit. This property can also be inferred from the sample path properties of the standard FBM (Fig. 3) simulated using the midpoint displacement algorithms, in comparison to the sample paths of the RL-FBM (Fig. 2) in the large-time asymptotic limit. The local regularity properties of the latter will approach the former when the large-time asymptotic is considered but the processes differ near the time origin. Since from the physical point of view, FBM cannot be made to start at $t=-\infty$, RL-FBM may turn out to be more appropriate in some applications, particularly in the modeling of anomalous diffusion where one usually considers the asymptotic process. Another advantage of RL-FBM is that it is defined for all $H>0$, thus it can be used for transport phenomena that are characterized by $H>1$.

IV. GENERALIZED LANGEVIN EQUATION APPROACH

A. Generalized Langevin equation

We shall first consider the Gaussian model proposed by Wang and co-worker [10,11]. They consider the following generalized Langevin equation for a particle of mass M:

$$\frac{dX(t)}{dt}=V(t), \tag{28}$$

$$M\frac{d^2X(t)}{dt^2}+M\int_0^t\lambda(t-\tau)V(\tau)d\tau=F(t), \tag{29}$$

where $\lambda(t-\tau)$ is the memory kernel of frictional force and $F(t)$ is a stationary Gaussian noise with zero mean and the long-range correlation property

$$\langle F(0)F(t)\rangle=F_0(\alpha)t^{-\alpha},\quad 0<\alpha<2. \tag{30}$$

With the help of the generalized second fluctuation-dissipation theorem, they obtained

$$\lambda(t)=\frac{F_0(\alpha)}{Mk_BT}t^{-\alpha}, \tag{31}$$

where T is temperature and k_B is Boltzmann's constant. By considering the large-time asymptotic condition, they obtained the following correlation function for the velocity process [11]:

$$\langle V(0)V(t)\rangle\sim(\alpha-1)t^{\alpha-2} \tag{32}$$

for $0<\alpha<1$ and $1<\alpha<2$. Equation (32) agrees with the correlation function for the fractional Gaussian noise associated with FBM if $\alpha=2H$. They proceeded to obtain a generalized Fokker-Planck equation for the PDF $P(x,t)$ for $X(t)$, which is basically the same as the effective Fokker-Planck equation (12) for $V(0)=0$ with some adjustments of constants. Thus the variance for the process $X(t)$ is given by $\langle X(t)^2\rangle\sim t^\alpha, t\to\infty$.

In the case of $\alpha=1$, Wang did not recover the usual diffusion equation for Brownian motion. Instead, the following asymptotic effective Fokker-Planck equation is obtained [11]:

$$\frac{\partial P(x,t)}{\partial t}=\frac{k_BT}{M}\ln t\frac{\partial^2P(x,t)}{\partial x^2} \tag{33}$$

with solution [subjected to $P(x,0)=\delta(x)$]

$$P(x,t)=\frac{1}{\sqrt{4\pi D_1 t(\ln t-1)}}\exp\left[-\frac{x^2}{4D_1 t(\ln t-1)}\right], \tag{34}$$

where $D_1=k_B T/M$. The variance has the power-logarithmic growth

$$\langle X(t)^2\rangle \sim t(\ln t-1), \quad t\to\infty. \tag{35}$$

They drew the conclusion that the generalized Langevin equation shows anomalous diffusion that is associated with FBM for $0<\alpha<1$ and $1<\alpha<2$; and the long-range correlation of the fluctuation force $F(t)$ is the physical origin of anomalous diffusion. For $\alpha=1$, one does not recover the normal diffusion, instead an anomalous diffusion with a mean-square displacement that varies with logarithmic time. This implies that $\alpha=1$ gives anomalous diffusion that is not related to FBM. A result similar to Eq. (35) was also obtained in [12,13].

We shall now show that the so-called anomaly mentioned above does not exist if the velocity process is regarded as a generalized random process. Let $V(t)$ be used to denote the continuous time derivative of $X(t)$. $V(t)$ cannot be considered pointwise for each t. Instead, it is a generalized function [14]:

$$V(\varphi)=\langle V,\varphi\rangle=\int_{-\infty}^{\infty}V(t)\varphi(t)dt \tag{36}$$

with $\varphi\in\mathcal{S}(R)$, the Schwarz space of test functions which satisfy

$$\lim_{|t|\to\infty}t^m\frac{d^n\varphi(t)}{dt^n}=0 \quad \text{for all positive integers } m,n. \tag{37}$$

Suppose V is a real-valued generalized random process with zero mean and correlation functional

$$C(\varphi,\psi)=\langle V(\varphi)V(\psi)\rangle=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\varphi(t)C_\alpha(t-s)\psi(s)dt\,ds, \tag{38}$$

where

$$C_\alpha(t)=\langle V(0)V(t)\rangle=c_\alpha|t|^{\alpha-2} \tag{39}$$

with $c_\alpha\sim\alpha(\alpha-1)$. Note that $C_\alpha(t)$ is locally integrable for $0<\alpha<1$. For $1<\alpha<2$, $C_\alpha(t)$ is given by the generalized function $c_\alpha\lceil t_+^{\alpha-2}\rceil$, where $\lceil(x_+^\rho)\rceil$ denotes the finite part of x_+^ρ, $-2<\rho<-1$. Here $\lceil(x_+^\rho)\rceil, -2<\rho<-1$, defines uniquely a homogeneous generalized function of degree ρ, whose restriction to $(-\infty,0)\cup(0,\infty)$ coincides with the function $|x|^\rho$. Noticing that $C_\alpha(t)$ has a simple pole at $\alpha=1$, we have in the sense of a generalized function, the limit

$$\lim_{\alpha\to1}c_\alpha|t|^{\alpha-2}\sim\delta(t), \tag{40}$$

where $\delta(t)$ is the Dirac δ function.

Now we consider the large-time asymptotic velocity as a generalized process, then its correlation function (32) has in the sense of a generalized function, the following limit for $\alpha=1$:

$$\lim_{\alpha\to1}\langle V(0)V(t)\rangle\sim\lim_{\alpha\to1}(\alpha-1)|t|^{\alpha-2}=\delta(t). \tag{41}$$

Then the effective Fokker-Planck equation (33) and its solution (34) now become the ordinary diffusion equation for Brownian motion with $\ln t$ and $t(\ln t-1)$ to be replaced by 1 and t, respectively. In other words, for $\alpha=1$ one recovers Brownian motion with $\langle X(t)^2\rangle\sim t$ instead of Eq. (35). It can be concluded that if proper care is taken to interpret the case of $\alpha=1$, the anomaly mentioned above does not exist. Thus asymptotically $(t\to\infty)$ the generalized Langevin equation of Wang and co-worker [10,11] provides a Gaussian model for the anomalous diffusion. The position process $X(t)$ resembles RL-FBM since it is assumed to start at $t=0$ and acquire the properties of FBM as $t\to\infty$. However, one cannot identify $X(t)$ with RL-FBM since its correlation function at intermediate times is not known. Due to this reason, such a Langevin approach to FBM is not unique as various possibilities may exist with different intermediate processes which have the same asymptotic limit process.

B. Fractional Langevin equation

Recall that the Ornstein-Uhlenbeck (OU) process $X_{OU}(t)$, which describes the Brownian particle in a harmonic oscillator potential, is the stationary solution of the Langevin equation

$$\left(\frac{d}{dt}+a\right)X_{OU}(t)=\eta(t), \quad a>0. \tag{42}$$

Brownian motion is recovered in the limit $a\to0$ or in the high frequency limit. Thus the OU process can be regarded as the stationary analog of Brownian motion. One would like to see whether the generalization of Eq. (42) to the fractional Langevin equation can give a solution $X_{OU}^\nu(t)$, which satisfies an analogous relation with the standard FBM. Consider first the following fractional Langevin equation :

$$(D^\nu+a)X_{OU}^\nu(t)=\eta(t), \quad \nu>0,a>0. \tag{43}$$

For $n-1<\nu<n, n>1$ and the following boundary conditions:

$$X_{OU}^\nu(0)=X_o, \quad \left.\frac{d^jX(t)}{dt^j}\right|_{t=0}=X_j, \quad j=1,\ldots,n-1, \tag{44}$$

the Laplace transform of Eq. (43) is

$$s^\nu\tilde{X}(s)+a\tilde{X}(s)=\tilde{\eta}(s)+\sum_{j=1}^{n}s^{\nu-j}X_{j-1}, \tag{45}$$

which gives

$$\tilde{X}(s)=\frac{\tilde{\eta}(s)}{s^{\nu}+a}+\sum_{j=1}^{n}X_{j-1}\frac{s^{\nu-j}}{s^{\nu}+a}. \tag{46}$$

The inverse Laplace transform gives the solution of Eq. (43):

$$X_{\rm OU}^{\nu}(t)=\sum_{j=1}^{n}X_{j-1}t^{j-1}E_{\nu,j}(-at^{\nu})+\int_0^t(t-u)^{\nu-1}E_{\nu,\nu}[-a(t-u)^{\nu}]\eta(u)du, \tag{47}$$

where $E_{\alpha,\beta}(z)$ is the generalized Mittag-Leffler function defined by [15]

$$E_{\alpha,\beta}(z)=\sum_{k=0}^{\infty}\frac{z^k}{\Gamma(\alpha k+\beta)},\quad \alpha>0,\beta>0. \tag{48}$$

For simplicity, one can let all X_j's equal to zero without affecting the conclusion to be drawn later on. Then, the covariance of $X_{\rm OU}^{\nu}(t)$ can be calculated for $s<t$ (see Appendix B):

$$\langle X_{\rm OU}^{\nu}(s)X_{\rm OU}^{\nu}(t)\rangle=\sum_{j,k=1}^{\infty}\frac{(-a)^{j+k-2}}{\Gamma(\nu j+1)\Gamma(\nu k)}s^{\nu j}t^{\nu k-1}\times {}_2F_1\left(1,1-\nu k,1+\nu j,\frac{s}{t}\right), \tag{49}$$

which shows that $X_{\rm OU}^{\nu}$ is nonstationary, hence it cannot be the stationary analog for FBM.

In order to see whether $X_{\rm OU}^{\nu}(t)$ can be used to describe the behavior of anomalous diffusion, one needs to consider its variance. It can be shown (see Appendix B) that for $t\to\infty$,

$$\langle [X_{\rm OU}^{\nu}(t)]^2\rangle\approx t^{-\nu-1}. \tag{50}$$

With $\nu=H+1/2$ and $1/2\leqslant H<1$, the variance of $X_{\rm OU}^{\nu}$ varies asymptotically as $t^{-H-3/2}$, which differs from t^{2H} of the anomalous diffusion. On the other hand, for $|at|\ll 1$ one gets

$$\langle [X_{\rm OU}^{\nu}(t)]^2\rangle\approx t^{2\nu-1}=t^{2H}. \tag{51}$$

This is expected as $a\to 0, X_{\rm OU}^{\nu}\to X_{\rm RL}$ as Eq. (43) reduces to the equation of RL-FBM.

Another way to fractionalize the Langevin equation is given by

$$(D+a)^{\nu}X_{\rm OU}^{\nu}(t)=\eta(t),\quad a>0,\nu>0. \tag{52}$$

Its stationary solution $X_{\rm OU}^{\nu}(t)$ is given by

$$X_{\rm OU}^{\nu}(t)=\int_{-\infty}^{\infty}G(x-u)\eta(u)du \tag{53}$$

with

$$G(t)=C(a,\nu)t^{\nu-1}e^{-at}\theta(t), \tag{54}$$

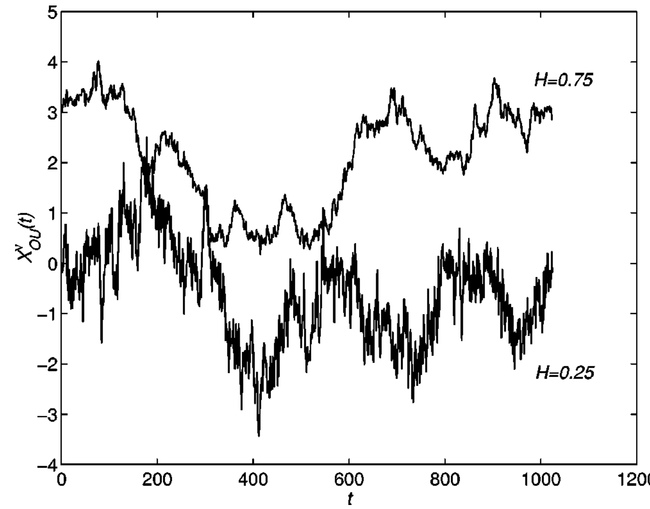

FIG. 4. The sample paths of fractional Ornstein-Uhlenbeck process for $H=0.25$ and $H=0.75$.

where $\theta(t)$ is the unit step function and $C(a,\nu)$ is a constant that depends on a and ν, which can be chosen as $C(a,\nu)=2^{-1+\nu/2}a^{\nu-1}[\Gamma(\nu)]^{-1}$. When $\nu=1$, $C(a,\nu)$ becomes unity. The covariance of the stationary process $X_{\rm OU}^{\nu}(t)$ is

$$\langle X_{\rm OU}^{\nu}(t+\tau)X_{\rm OU}^{\nu}(t)\rangle=\frac{a^{\nu-3/2}}{\sqrt{2\pi}}|\tau|^{\nu-1/2}K_{\nu-1/2}(|a\tau|), \tag{55}$$

where $K_{\nu}(z)$ is the modified Bessel function of the second kind (or Macdonald function) of order ν. Its spectral density is $2^{\nu-1}a^{2\nu-2}\Gamma(\nu)(a^2+\omega^2)^{-\nu}$ [16], p. 464, Eq. (3771.2)], which gives the spectral density for OU process $\sim(a^2+\omega^2)^{-1}$ when $\nu=1$.

By using the following asymptotic property of the modified Bessel function:

$$K_{\nu}(z)\sim\frac{\Gamma(\nu)}{2}\left(\frac{z}{2}\right)^{-\nu}\quad \text{for}\quad z\to 0, \tag{56}$$

and the symmetric property $K_{\nu}(z)=K_{-\nu}(z)$, one can verify from the covariance (55) that for $|a\tau|\ll 1$,

$$\langle [X_{\rm OU}^{\nu}(t+\tau)-X_{\rm OU}^{\nu}(t)]^2\rangle=\frac{\sqrt{\pi/2a^2}}{\sin[(\nu-1/2)\pi]\Gamma(\nu+1/2)}|a\tau|^{2\nu-1}, \tag{57}$$

which is similar to the variance of the increment process for standard FBM with $\nu=H+1/2$. In the high frequency regime with $\omega\gg a$, the spectral density scales as $\sim\omega^{-2\nu}$ or $\omega^{-(2H+1)}$. Equation (57) together with the Wiener-Khinchine theorem, which relates the covariance of a stationary process to the power spectral density, allows one to simulate the sample paths (Fig. 4) of the fractional Ornstein-Uhlenbeck process using an algorithm based on spectral technique [17]. The stationary properties of the process are evident from the graphs as there exists no obvious trend in the sample paths in contrast to the upward or downward trends observed in Figs. 2 and 3. From the above discussion, we see that Eq. (52) is the appropriate Langevin equation which gives the fractional Ornstein-Uhlenbeck process or the stationary analog of FBM.

V. FIRST PASSAGE TIME DISTRIBUTION FUNCTION

It has been shown earlier that three processes, namely, SBM and two versions of FBM, satisfy the same effective Fokker-Planck equation (up to a multiplicative constant). These processes have quite different properties and they satisfy free Langevin-type equations (5) and (25) with different noise sources and the free fractional Langevin equation (16). The fact that different Langevin equations give rise to the same effective Fokker-Planck equation implies that the former contain more information than the latter. In general, the Fokker-Planck equation describes the process fully only if the process is Markovian. We shall show in this section that in the determination of the first passage time (FPT) distribution the effective Fokker-Planck equation (12) can be used for the Markovian SBM, whereas it fails to apply to the non-Markovian FBM. However, the FPT distribution of SBM can be used to obtain bounds for the FPT distributions of RL-FBM and standard FBM with the help of the Slepian theorem [18].

An interesting problem in the theory of random processes is to determine how long a particle remains in a certain region x, where its position is described by a diffusion (or Fokker-Planck) equation. This leads us to consider the FPT denoted by T_a, which is the time taken for the process to reach $x=a$ for the first time, having started from x_o at $t=0$ [19]. One has

$$T_a=\inf\{t>0 \mid X(t)=a\}. \tag{58}$$

Clearly FPT is a random variable which varies from realization to realization. It can only be determined exactly for a few simple cases, which include the Brownian motion. In this section, we intend to use inequalities in the covariances of SBM, and the two versions of FBM to obtain an inequality for their first passage time distributions.

In the case of SBM $X_*(t)$ we can follow the same method for Brownian motion to obtain the distribution function for its FPT [19]. The time T_a for $X_*(t)$ to hit the level a first will be less than t iff $M(t)=\sup_{0\leqslant s\leqslant t}X_*(s)$, in that time is at least a. Thus for $t>0$,

$$\begin{aligned}P\{M(t)\geqslant a\}&=P\{T_a\leqslant t\}\\&=2P\{X_*(t)\geqslant a\}\\&=\frac{1}{\sqrt{\pi D t_*}}\int_a^\infty \exp\left[-\frac{x^2}{4t_*}\right]dx\\&=\frac{1}{\sqrt{\pi D}}\int_{a/\sqrt{t_*}}^\infty \exp\left[-\frac{y^2}{4}\right]dy. \end{aligned}\tag{59}$$

By changing the variable $s=a^2 t_*/x^2$, the distribution function for FPT is

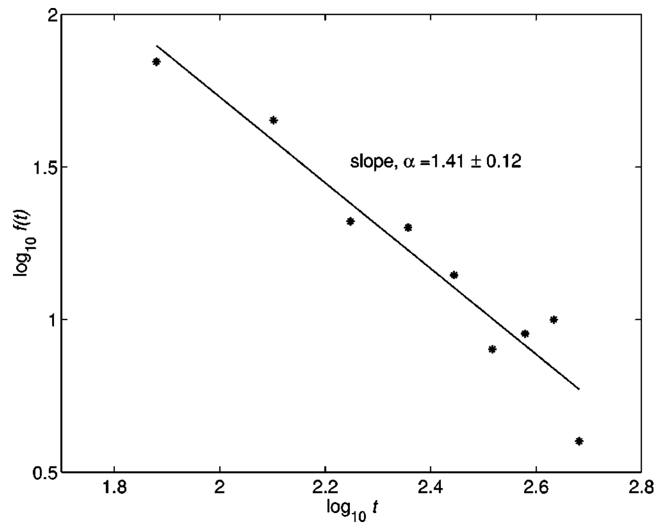

FIG. 5. Estimation of the scaling exponent α of the first passage time distribution $f(t)\sim t^{-\alpha}$, where $\alpha=H+1$ for the rescaled Brownian motion.

$$F(t)=P\{T_a\leqslant t\}=\frac{a}{2\sqrt{\pi D}}\int_0^{t_*} s^{-3/2}\exp\left[-\frac{a^2}{4s}\right]ds. \tag{60}$$

The distribution density $f(t)$ of T_a is then given by

$$f(t)=\frac{dF(t)}{dt}=\frac{Ha}{\sqrt{\pi D}t^{H+1}}\exp\left[-\frac{a^2}{4t^{2H}}\right]. \tag{61}$$

When $H=1/2$, the FPT distribution density for Brownian motion is recovered. As $t\to\infty$, $f(t)$ decays as $t^{-(H+1)}$ and this is illustrated in Fig. 5, which shows the result of the FPT estimation using 1000 realizations for the case when $H=0.4$. The estimated value of $H=0.41\pm0.12$ is in agreement with the calculated value despite the small number of the realizations considered.

Alternatively, the FPT distribution of $X_*(t)$ can be determined by considering the effective Fokker-Planck equation with appropriate boundary conditions [20]. Since we are interested in first arrival time, we consider the process up to that time and then kill it by absorption. In other words, one works with an absorbed process, with absorbing boundaries at $x=-\infty$ and $x=a$. Due to the symmetry of the $P(x,t)$ under consideration, and by changing the variable $x\to a-x$, the necessary boundary conditions become

$$P(0,t)=0,\qquad P(\infty,t)=0,$$
$$P(x,0)=\delta(x-a). \tag{62}$$

With these boundary conditions, the solution to the effective Fokker-Planck equation for FBM is given by

$$P_a(x,t)=P(x,t|a,0)-P(x,t|-a,0), \tag{63}$$

where $P(x,t|a,0)$ is the PDF in the absence of boundaries for the position at time t of a particle initially at a. Then

$$P_a(x,t)=\frac{1}{\sqrt{4\pi D}t^H}\left[\exp\left(-\frac{(x-a)^2}{4Dt^{2H}}\right)-\exp\left(-\frac{(x+a)^2}{4Dt^{2H}}\right)\right]. \tag{64}$$

Let $S(t)$ denote the survival probability, that is, the probability that the diffusing particle does not reach a until time t. Then

$$S(t)=\int_a^\infty P_a(x,t)dx.$$

The FPT distribution function $F(t)=1-S(t)$, and the distribution density for the FPT is given by

$$\begin{aligned} f(t)&=-\frac{d}{dt}\int_0^\infty P_a(x,t)dx \\ &=-\frac{d}{dt}\left[\frac{1}{\sqrt{\pi}}\left(\int_{-a/\sqrt{4D}t^H}^\infty e^{-u^2}du-\int_{a/\sqrt{4D}t^H}^\infty e^{-v^2}dv\right)\right], \end{aligned} \tag{65}$$

where $u=(x-a)/\sqrt{4D}t^H$ and $v=(x+a)/\sqrt{4D}t^H$. Again one gets Eq. (61).

Note that the generalized diffusion equation and Fokker-Planck equation (with appropriate boundary conditions) are the most commonly used mathematical tools for the determination of FPT distribution. However, due to its non-Markovian character, FBM is not fully characterized by the effective Fokker-Planck equation (12). Various attempts to obtain a Fokker-Planck or generalized master equation which can provide a correct description of FBM have so far been unsuccessful. We remarked that, in general, the Langevin equation contains more information than the corresponding Fokker-Planck equation. It is possible to obtain the same information from the Langevin equation and the Fokker-Planck equation in the case of a Markov process. In the case of non-Markovian Gaussian FBM, correlation at different times can be obtained from the free fractional Langevin equations (16) and (25) but not from the effective Fokker-Planck equation (12). In fact, FBM is highly non-Markovian and there does not exist a finite-dimensional supplementary variable representation of FBM which makes it Markovian. As a result of the intrinsically non-Markovian character of FBM, the determination of its FPT distribution becomes difficult and so far no exact result has been obtained. Various methods have been used to determine the large-time limit of the FPT distribution of FBM. These include the distribution of the maximum of a FBM [21] and the level crossing and first return time [22,23]. The result obtained for the FPT distribution density in the large-time limit varies as $t^{-(2-\alpha/2)}$ [or $t^{-(2-H)}$], which has been verified by computer experiments [23,24]. When $\alpha=1$ (or $H=1/2$), one gets exactly the result for Brownian motion. Note that in all these methods of estimating FPT distribution probability, the stationary property of the increment process of FBM played a crucial role.

Since the FPT distribution of SBM is known exactly, one can apply the comparison theorem of Slepian [18] to obtain bounds for the FPT distributions for RL-FBM X_{RL} and standard FBM X_{W}. $C_*(s,t)$, $C_{\mathrm{RL}}(s,t)$, and $C_{\mathrm{W}}(s,t)$ denote the correlation functions of X_*, X_{RL}, and X_{W}, respectively. Suppose these three centered Gaussian processes are appropriately normalized such that their variances are equal. Since their correlation functions satisfy the following inequalities for $s,t\geqslant 0$ (see Appendix C for proof):

$$C_*(s,t)\leqslant C_{\mathrm{RL}}(s,t)\leqslant C_{\mathrm{W}}(s,t) \quad \text{for} \quad 1/2\leqslant H<1 \tag{66}$$

and

$$C_{\mathrm{RL}}(s,t)\leqslant C_{\mathrm{W}}(s,t)\leqslant C_*(s,t) \quad \text{for} \quad 0<H\leqslant 1/2, \tag{67}$$

then according to the Slepian theorem their FPT distributions satisfy the following inequalities for $t\geqslant 0$:

$$F_{\mathrm{W}}(t)\leqslant F_{\mathrm{RL}}(t)\leqslant F_*(t) \quad \text{for} \quad 1/2\leqslant H<1 \tag{68}$$

and

$$F_*(t)\leqslant F_{\mathrm{W}}(t)\leqslant F_{\mathrm{RL}}(t) \quad \text{for} \quad 0<H\leqslant 1/2. \tag{69}$$

Since for large t, $X_{RL}\to X_{\mathrm{W}}(t)$ and thus $F_{\mathrm{W}}(t)\approx F_{\mathrm{RL}}(t)$ asymptotically. When appropriately normalized, equality holds when $H=1/2$ in the above equations.

VI. MULTIFRACTIONAL GENERALIZATIONS

Many transport phenomena such as anomalous diffusion in certain heterogeneous media have a far more complex scaling behavior than simple fractals. Disordered porous materials are seldom heterogeneous or irregular in a uniform sense; they usually contain multiple, nested natural length and time scales or continuously evolving scales. Local porosity models are often used to study transport properties in such media [25]. Another example is hydraulic conductivities that display increasing heterogeneity at decreasing scales [26]. Such multifractal conductivities have an important effect on contaminant transport in the subsurface. Last but not least, the classic example offered by the dynamical processes associated with turbulent cascades, which are multifractal rather than monofractal. The description of multifractal cascade processes, in general, require an infinite hierarchy of scaling exponents for its characterization.

Monofractal models with a single scaling parameter presented earlier are inadequate for such processes that display multifractal features, in the sense that their "irregularities" can fluctuate from point to point in the media. To describe these multifractal phenomena, one possible way is to generalize the Hurst exponent so that it becomes a local quantity:

$$|X(t+\tau)-X(t)|\sim\tau^{H(t)} \tag{70}$$

for τ sufficiently small. This local Hurst exponent $H(t)$ can then be regarded as the Hurst exponent of $X(t)$ at the point t. Therefore, one can characterize local heterogeneity with different local power-law scaling using the time- (or space-) dependent Hurst exponents.

The commonly used multifractal analysis was the one first introduced by Frisch and Parisi [27] based on the distribution of singularities in multifractal measures for modeling energy dissipation in turbulent fluids. Such a method has been further developed with the help of wavelet analysis [28]. Multifractal analysis is widely used to model multifractal transport processes such as anomalous diffusion in multifractal porous media [29], random fractals [30] and percolation clusters [31], hydraulic conductivity distribution [26], and other multifractal transport phenomena. In this section, we shall adopt a different approach, which deals directly with some Gaussian multifractal processes.

A. Multifractional Brownian motion

We shall first consider the generalization of FBM to the multifractional Brownian motion (MBM). The two versions of FBM, the standard FBM X_{W} and the RL-FBM X_{RL}, can be extended to their respective MBMs Y_{W} and Y_{RL} by replacing the Hurst exponent H by a time- (or position-) dependent function $H(t)$ in Eqs. (19) [32] and (22′) [33,34]. $H(t)$ is assumed to be a smooth function with $0<H(t)<1$.

Due to the fact that the Hurst exponent is not a constant any more, one expects that the MBMs would not preserve the global properties of the FBMs, such as stationary increments and self-similarity. However, these properties can still hold locally. It can be shown easily that the increments of Y_{W} are locally stationary, or to be more exact, locally asymptotically stationary. The variance of the increment process satisfies

$$\langle [Y_{\mathrm{W}}(t+\tau)-Y_{\mathrm{W}}(t)]^2\rangle=\sigma_{H(t)}|\tau|^{2H(t)}, \quad \tau\to 0, \tag{71}$$

where $\sigma_{H(t)}$ is dependent on $H(t)$. The covariance of the standard MBM and RL-MBM can be calculated [32]. However, for the purpose of local properties it will suffice to consider the local covariance which is the same for both versions of MBM [35]. By assuming that $H(t)$ is smooth such that $H(t+\tau)\simeq H(t)$ for $\tau\to 0$, the local covariance can be calculated and is given by

$$\langle Y_{\mathrm{W}}(t+\tau)Y_{\mathrm{W}}(t)\rangle=\frac{\sigma_{H(t)}}{2}[|t+\tau|^{2H(t)}+|t|^{2H(t)} -|\tau|^{2H(t)}], \quad \tau\to 0. \tag{72}$$

The increments of RL-MBM also satisfy the locally asymptotically stationary property, hence its local covariance has the same form as Eq. (72) (up to a multiplicative deterministic function of time). It is interesting to note that when extended to MBM, the advantage of the standard FBM over RL-FBM, namely, the stationarity of increments disappears and the two versions of MBMs have very similar properties.

In order to give an appropriate definition of local self-similarity, recall that the increments of a self-similar process $X(t)$ are self-similar provided that the increments are stationary. Then for $r>0$,

$$X(t+\tau)-X(t)=r^{-H}[X(t+r\tau)-X(t)]. \tag{73}$$

For increments that are locally asymptotically stationary, one has the following characterization of local self-similarity. The standard MBM $Y_{\mathrm{W}}(t)$ is indexed by $H(t) \in C^{\gamma}(R,(0,1)), t\in R$ for some positive γ with $\gamma>\sup H(t)$, then it can be shown that $Y_{\mathrm{W}}(t)$ is said to satisfy the locally asymptotically self-similar property if

$$\lim_{\rho\to 0^+}\left(\frac{Y_{\mathrm{W}}(t_o+\rho u)-Y_{\mathrm{W}}(t_o)}{\rho^{H(t_o)}}\right)_{u\in R}=[X_{H(t_o)}(u)]_{u\in R}, \tag{74}$$

where the equality in law is up to a multiplicative deterministic function of time and $X_{H(t_o)}$ is the standard FBM indexed by $H(t_o)$. Equation (74) holds also for the RL-MBM if Y_{W} and $u\in R$ are replaced by Y_{RL} and $u\in R_+$, respectively [32]. This property can be verified by using the local covariance (72). One can interpret Eq. (74) as the existence of a tangent FBM $X(t_o)$ at each time t_o where the MBM is defined. The Hurst exponent of this local FBM is $H(t_o)$.

For applications to anomalous diffusion processes that exhibit multifractal features, the following characterization of the local property of MBM can be useful. To be specific, let us consider the RL-MBM (it applies to standard MBM as well). Let $H_\epsilon(t)=H(t/\epsilon), \sigma_{H_\epsilon(t)}=\sigma_{H(t/\epsilon)}$, and

$$Y_{H_\epsilon(t)}(t)=\frac{1}{\Gamma(H_\epsilon(t)+1/2)}\int_0^t (t-u)^{H_\epsilon(t)-1/2}\eta(u)du. \tag{75}$$

The variance of the increment process of $Y_{H_\epsilon(t)}$ is

$$\langle [Y_{H_\epsilon(t)}(t+\tau)-Y_{H_\epsilon(t)}(t)]^2\rangle\approx D_{H_\epsilon(t)}|\tau|^{2H_\epsilon(t)} \tag{76}$$

for ϵ sufficiently small such that the increment process is stationary over $\tau\ll\epsilon^{-1}$ and also we have assumed $H_\epsilon(t+\tau)\simeq H_\epsilon(t)$. One can regard the parameter ϵ as a measure of stationarity since it determines the size of the neighborhood of t for which the increments of $Y_{H_\epsilon(t)}$ are approximately stationary. In other words, $Y_{H_\epsilon(t)}$ behaves locally like FBM with the Hurst exponent frozen at t_o for scales that are smaller than the interval of stationarity. Based on the resampling algorithm mentioned in [36], the sample path of RL-MBM is shown in Fig. 6 for a particular choice of time-varying function, $H(t)=a\exp(-bt^2)+c$, where a,b,c are arbitrarily chosen parameters. Details of the simulation algorithms are given in Appendix A.

Finally, we consider the possibility of describing MBM by fractional stochastic differential equations analogous to Eqs. (16) and (25). Note that although the usual fractional calculus is well suited for the description of anomalous diffusion, it is not applicable if the diffusion occurs in multifractal media with a fractional exponent that depends on time (or space). Thus it is necessary to generalize the usual fractional calculus. One way to do this is to consider a fractional derivative and fractional integral of variable order. A direct generalization of the RL-fractional integration and differentiation to variable order $\beta(t)$ is [37,38]

$$I^{\beta(t)}f(t)=\frac{1}{\Gamma(\beta(t))}\int_0^t (t-u)^{\beta(t)-1}f(u)du, \quad \beta(t)>0 \tag{77}$$

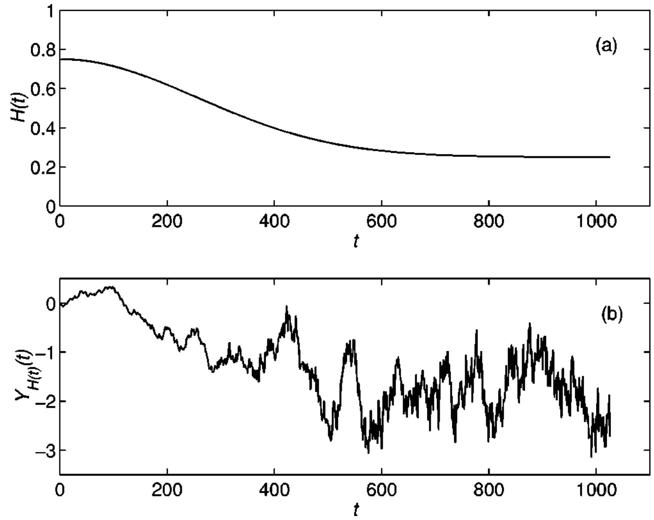

FIG. 6. (a) The time-varying Hurst exponent $H(t) = 0.5\exp(-t^2)+0.25$ and (b) the corresponding sample path of RL-MBM.

and the fractional differentiation of variable order $\beta(t)$, $0<\beta(t)<1$:

$$\mathcal{D}^{\beta(t)}f(t)=\frac{1}{\Gamma(\beta(t)-1)}\frac{d}{dt}\int_0^t(t-u)^{-\beta(t)}f(u)du,$$

$$0<\beta(t)<1. \tag{78}$$

Equation (77) gives RL-MBM if $f(t)=\eta(t)$ and $\beta(t)=H(t)+1/2$. However, in contrast to the case $\beta(t)=\beta$, it is not possible to obtain a stochastic equation of variable order for $Y_{RL}(t)$ analogous to Eq. (16) by inverting Eq. (77). The reason is that Eq. (78) is not the left inverse of the operator $I^{\beta(t)}$, that is,

$$\mathcal{D}^{\beta(t)}I^{\beta(t)}f(t)\neq f(t), \tag{79}$$

which can be verified by direct computation for some simple functions [37,38]. Much work needs to be done to derive a stochastic fractional differential equation for MBM.

B. Multifractional Ornstein-Uhlenbeck process

It may be interesting to find out whether the link between the fractional OU process and the standard FBM still holds when extended to the multifractional case. For this purpose we need to extend $X^{\nu}_{\mathrm{OU}}(t)$ to the multifractional $X^{\nu(t)}_{\mathrm{OU}}(t)$, which is given by Eq. (53) with ν replaced by $\nu(t)>0$. The multifractional OU process is a nonstationary process. Its covariance is rather in a complicated form, which can be expressed in terms of the confluent hypergeometric function ${}_1F_1(\alpha,\gamma,z)$:

$$\begin{aligned}\langle X^{\nu(s)}_{\mathrm{OU}}(s)X^{\nu(t)}_{\mathrm{OU}}(t)\rangle=&\frac{C(a,\nu(s))C(a,\nu(t))e^{-a(s-t)}}{\Gamma(-\nu(s))(2a)^{1+\nu(s)+\nu(t)}}\\&\times\{\Gamma(-\nu(s))\Gamma(1+\nu(s)+\nu(t))\\&\times{}_1F_1(-\nu(s),-\nu(s)-\nu(t),2a(s-t))\\&+(2a(s-t))^{1+\nu(s)+\nu(t)}\Gamma(1+\nu(t))\\&\times\Gamma(-1-\nu(s)-\nu(t))\,{}_1F_1(1+\nu(t),\\&\times 2+\nu(s)+\nu(t),2a(s-t))\}.\end{aligned} \tag{80}$$

If $\nu(t)$ is assumed to be a smooth function, then $\nu(s)\simeq\nu(t)$ for $|t-s|=\tau\ll 1$. The local covariance of the multifractional OU process can be shown to be

$$\begin{aligned}\langle X^{\nu(s)}_{\mathrm{OU}}(t)X^{\nu(t)}_{\mathrm{OU}}(t+\tau)\rangle=&C^2(a,\nu(t))\tau^{\nu(t)-1/2}K_{\nu(t)-1/2}(a\tau)\\&\approx\frac{\sqrt{(\pi/2)a^2}}{\sin\{[\nu(t)-1]\pi\}\Gamma(\nu(t)+1/2)}\\&\times|a\tau|^{2\nu(t)-1}\end{aligned} \tag{81}$$

for $\tau\ll 1$. Thus $X^{\nu(t)}_{OU}(t)$ is a locally asymptotically stationary process. In other words, it behaves like the fractional OU process indexed by $\nu(t)$. Therefore one can conclude that the link between the standard FBM and fractional OU process is preserved locally when extended to their corresponding multifractional process.

C. Time-rescaled Brownian motion with variable scaling

Finally, we consider the generalization of SBM by replacing the constant scaling exponent α by a variable scaling $\alpha(t)$:

$$X_{\alpha(t)}(t)=X(t^{\alpha(t)}), \tag{82}$$

where $\alpha(t)$ is assumed to be a smooth function with $0<\alpha(t)<2$. In terms of white noise, one has

$$X_{\alpha(t)}(t)=\int_0^t u^{\alpha(t)-1/2}\eta(u)du. \tag{83}$$

The covariance of $X_{\alpha(t)}$ is

$$\langle X_{\alpha(t)}(t)X_{\alpha(s)}(s)\rangle=t^{\alpha(t)}\wedge s^{\alpha(s)}. \tag{84}$$

First we note that the Markov property is preserved for $X_{\alpha(t)}(t)$, provided $\alpha(t)$ is a monotonic increasing function such that the time ordering will not be changed by the time scaling $t\to t^{\alpha(t)}$. Due to the time-dependent scaling exponent, properties of $X_*(t)$ such as independent increments and self-similarity are lost. However, one can still hope that these properties may hold locally, that is, for a fixed t_o, $X_{\alpha(t_o)}(t_o)$ behaves like $X_*(t_o)$ with a scaling exponent $\alpha(t_o)$. For nonoverlapping intervals $(s,s+\tau_1)$ and $(t,t+\tau_2)$ with $\tau_1,\tau_2>0$, one has $\alpha(s+\tau_1)\simeq\alpha(s)$, $\alpha(t,t+\tau_2)\simeq\alpha(t)$ for $\tau_1\ll s$, $\tau_2\ll t$. The covariance of the increment process is

$$\langle [X_{\alpha(s)}(s+\tau_1)-X_{\alpha(s)}(s)][X_{\alpha(t)}(t+\tau_2)-X_{\alpha(t)}(t)]\rangle$$
$$=(s+\tau_1)^{\alpha(s)}\wedge(t+\tau_2)^{\alpha(t)}-(s+\tau_1)^{\alpha(s)}\wedge t^{\alpha(t)}-s^{\alpha(s)}\wedge(t+\tau_2)^{\alpha(t)}+s^{\alpha(s)}\wedge t^{\alpha(t)}, \quad (85)$$

which vanishes for either $s>t$ or $s<t$ if $\alpha(t)$ is a monotonic function. Thus the increments of $X_{\alpha(t)}(t)$ are asymptotically locally independent for nonoverlapping intervals.

In contrast to the standard MBM, the absence of locally stationary increments for $X_{\alpha(t)}(t)$ rules out the use of Eq. (74) to characterize a locally asymptotic self-similarity. In fact, precisely due to this reason, the time-rescaled Brownian motion of variable order does not satisfy self-similarity locally. To characterize the self-similar property over a very short interval, it is necessary to consider the increment process over such an interval. Let $(t_o,t_o+\tau_1),(t_o+\tau_2)$ be two overlapping intervals with $\tau_1,\tau_2>0$ and $\tau_1,\tau_2\ll t_o$. Since $\alpha(t)$ is smooth, $\alpha(t_o+\tau_1)\simeq\alpha(t_o)\simeq\alpha(t_o+\tau_2)$. Then one has

$$\langle [X_{\alpha(t_o)}(t_o+\tau_1)-X_{\alpha(t_o)}(t_o)][X_{\alpha(t_o)}(t_o+\tau_2)-X_{\alpha(t_o)}(t_o)]\rangle$$
$$=(t_o+\tau_1\wedge\tau_2)^{\alpha(t_o)}-t_o^{\alpha(t_o)}. \quad (86)$$

No matter how small τ_1 and τ_2 are, any scaling by $r>0$ inevitably leads to the exponent $\alpha(rt_o)$, thus denying $X_{\alpha(t)}$ to satisfy the condition for a locally asymptotic self-similarity. As a result $X_{\alpha(t)}$ is unsuitable for modeling multifractal transport phenomena which satisfy local self-similarity.

VII. BEYOND GAUSSIAN MODELS

There are empirical evidences indicating that there exist non-Gaussian anomalous diffusion processes [1–3], which includes diffusion with jumps. We shall comment briefly on some common non-Gaussian models and their possible connection with the Gaussian models.

As RL-FBM is the solution of the fractional Langevin equation for a free particle, it is natural to consider the diffusion equation with fractional time derivative as follows:

$$\frac{\partial P(x,t)}{\partial t}=D_\alpha\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^2 P(x,t)}{\partial x^2}, \qquad 0<\alpha<2. \quad (87)$$

Its solution is a non-Gaussian PDF which can be associated to a continuous time random walk [1]. It is a symmetric PDF and for large x, each branch of $x>0$ and $x<0$ exhibits exponential decay in the "stretched" variable $|x|^{2/(2-\alpha)}$:

$$P(x,t)\sim g(t)|x|^{(\alpha-1)/(2-\alpha)}\exp[-h(t)|x|^{2/(2-\alpha)}] \quad (88)$$

for $|x|\gg t^{\alpha/2}$, where $g(t)$ and $h(t)$ are certain positive functions of t. This non-Gaussian PDF satisfies the anomalous diffusion relation (1). In the limit $t^\alpha/x^2\gg 1$, the leading terms for the non-Gaussian PDF and the Gaussian PDF (10) have the same time dependence $\sim t^{-\alpha/2}$.

The other non-Gaussian process widely used to model anomalous diffusion is the Levy stable process [2,3]. Such a Markov jump process can be associated with the fractional-space diffusion equation

$$\frac{\partial P(x,t)}{\partial t}=D\nabla^\mu P(x,t), \quad (89)$$

where ∇^μ denotes the Riesz fractional derivative:

$$\nabla^\mu=-\int\frac{dk}{2\pi}e^{-ikx}|k|^\mu, \qquad 0<\mu<2. \quad (90)$$

The solution of Eq. (89) in the Fourier space gives the symmetric Levy distribution in the form $P(k,t)\sim\exp[D|k|^\mu]$. It has the heavy tailed behavior in x space for $x^\mu\gg 1$:

$$P(x)\sim\frac{1}{|x|^{1+\mu}}. \quad (91)$$

One shortcoming of the Levy process is that its variance is infinite (in fact, all nth moments with $n>\alpha$ are infinite). This leads to a difficulty in terms of physical interpretation, in particular, when applied to the case of enhanced diffusion (superdiffusion). However, there are ways to overcome this problem. For example, the truncated Levy process with values of $P_L(x)$ vanishing outside some specified "length." One can also impose restrictions on the spatiotemporal stepping distributions or on velocities of the particles. Such conditions, of course, will alter the Markovian character of the original process.

The Levy stable process is a μ stable, $(1/\mu)$-self-similar process with independent increments. Note that, in general, Levy processes are multifractal; this is true when their measure is neither too small nor too large near zero [39]. However, for application to non-Gaussian anomalous diffusion with variable exponents, it may be useful to generalize Levy processes to stablelike processes by allowing variable μ. Bass [40] constructed a one-dimensional stablelike process using the (one-dimensional analog of the) pseudodifferential operator $-(-\Delta)^{\mu(t)/2}$ of variable order of differentiation as its generator. Here $\mu(t)$ is required to satisfy some mild conditions such as the continuity and regularity condition $0<\inf_t\mu(t)\leq\sup_t\mu(t)<2$. This generalized stablelike process behaves locally like a symmetric Levy stable process, i.e., for a fixed t_o, the process is a symmetric $\mu(t_o)$-stable process.

A non-Gaussian generalization of FBM that preserves its H-self-similar property and the stationary of its increments is the linear fractional Levy motion, which can be defined as [41]

$$X_{\mu,H}(t)=\int_{-\infty}^{\infty}[|t-u|^{H-1/\mu}-|u|^{H-1/\mu}]dL_\mu(u), \quad (92)$$

where L_μ is an H-self-similar, μ-stable measure. Such a process may provide more flexibility as far as applications are concerned since it is characterized by two parameters H and μ. However, it still suffers the same problem as the Levy stable process, i.e., it has infinite variance. Finally, one can also generalize the H exponent to a time varying function $H(t)$ to obtain the multifractional Levy-motion; this process will be discussed elsewhere.

VIII. DISCUSSION AND CONCLUSIONS

There exist several random processes that satisfy the anomalous diffusion relation (1). Three such processes, namely, SBM, RL-FBM, and standard FBM, which are all Gaussian and self-similar are considered. Their properties differ considerably, ranging from the Markov property and independent increments for SBM to the stationary and nonstationary increments for the non-Markov standard FBM and RL-FBM, respectively. As there exist a number of different mechanisms leading to the anomalous diffusion, so there is also a need to have several different random processes to describe these anomalous diffusive motions. It is necessary to know additional conditions, both empirical as well as theoretical, in order to determine the appropriate random process to be used for a particular system that undergoes anomalous diffusion. The model adopted not only has to describe correctly the asymptotic equilibrium state, it needs to be able to portray the intermediate stages as well. Thus a better understanding of the physical mechanism of the microscopic motion for anomalous diffusion is necessary in order to identify the appropriate model.

As far as these three Gaussian processes are concerned, a useful way to verify the suitability of one of them for modeling anomalous diffusion is the knowledge of FPT distribution. The FPT distribution for SBM and standard FBM are different, even though they have the same PDFs. In fact, the connection between the FPT and PDF of a random process, in general, can be quite complicated. Even a complete knowledge of the PDF may not be able to determine the FPT distribution, as in the case of FBM. Since only the FPT distribution of SBM is known exactly among the three Gaussian processes, one can apply the Slepian theorem to compare the FPT of SBM, and the two FBMs. This provides the upper bound (for $0<H\leqslant 1/2$) and lower bound ($1/2\leqslant H<1$) for the FPT distributions of the two FBMs.

Finally, we note that multifractional generalizations of FBM and SBM show that the former still preserves the properties of FBM locally, whereas the latter does not preserve the self-similarity locally. Thus, only MBM and the multifractional OU process can be regarded as candidates for Gaussian models for anomalous diffusion with variable scaling exponents.

ACKNOWLEDGMENTS

This work was supported by the Malaysian Ministry of Science and Technology under IRPA Grant No. 09-02-02-0092. We thank Professor M. Ding, Professor G. Rangarajan, and Professor J. Krug for correspondences; and Professor S. G. Samko, Professor G. M. Molchan, and Professor A. Hansen for sending us their papers.

APPENDIX A

The sample paths of the rescaled Brownian motion are obtained by considering the discrete version of Eq. (4) for discrete time $t_j = j\Delta$, $j\in Z^+$ and time step $\Delta t = 1/(N-1)$:

$$X_*(t)=\sum_{i=1}^{j}\int_{(i-1)\Delta t}^{i\Delta t}\tau^{\alpha-1/2}dB(\tau). \tag{A1}$$

Note that $dB(\tau)=\eta(\tau)d\tau$ is the increment of Brownian motion, thus one can approximate

$$dB(\tau)=\left(\frac{\eta_i}{\sqrt{\Delta t}}\right)d\tau, \tag{A2}$$

where η_i is the discrete sequence of Gaussian white noise with zero mean and unit variance. Thus, Eq. (A1) is reduced to

$$X_*(t_j)\simeq\sum_{i=1}^{j}\frac{\eta_i}{(\alpha+1/2)}[(i)^{\alpha+1/2}-(i-1)^{\alpha+1/2}](\Delta t)^{\alpha}, \tag{A3}$$

which forms the generator of the sample paths shown in Fig. 1.

The simulation of RL-FBM is carried out based on the similar algorithms as described above but using the following approximation of Eq. (19):

$$X_H^{\mathrm{RL}}(t_j)=\frac{1}{\Gamma\left(H+\frac{1}{2}\right)}\sum_{i=1}^{j}\int_{(i-1)\Delta t}^{i\Delta t}(t_j-\tau)^{H-1/2}dB(\tau). \tag{A4}$$

Upon integrating Eq. (A4) gives

$$X_H^{\mathrm{RL}}(t_j)=\sum_{i=1}^{j}\left(\frac{\eta_i}{\sqrt{\Delta t}}\right)w_{j-i+1}\Delta t, \tag{A5}$$

with the modified weighting function as suggested in [42],

$$w_i=\frac{1}{\Gamma(H+1/2)}\left[\frac{t_i^{2H}-(t_i-\Delta t)^{2H}}{2H\Delta t}\right]^{1/2}, \tag{A6}$$

to give the accurate scaling of the variance, i.e., $\mathrm{var}[X_H(t_j)]\sim t_j^{2H}$. The sample paths in Fig. 2 are simulated using the generator given in Eq. (A5). There exist a number of well-known techniques for the simulation of the standard FBM, such as the random midpoint displacement method [43] and the wavelet-based algorithms [44,45], these will not be described here.

A discrete sequence of N points RL-MBM, $Y_{H(t_j)}(t_j)$ with time sequence $H(t_j)$ is obtained by sampling the points, namely, $Y_{H(t_j)}(t_j)=X_{H(t_j)}^{\mathrm{RL}}(t_j)_+, 0\leqslant j\leqslant N$ from a set of N-sample paths of RL-FBM generated for the respective pointwise values of $H(t_j)$ evaluated at $t_j=j/(N-1)$. For a particular choice of $H(t)$ as shown in Fig. 6(a), the sample path with the prescribed local regularity is shown in Fig. 6(b). A simple method for numerical estimation of $H(t)$ is described in [33,36].

APPENDIX B

The covariance of the process $X_{\mathrm{OU}}^{\nu}(t)$ can be calculated as follows:

$$\langle X_{\mathrm{OU}}^{\nu}(s)X_{\mathrm{OU}}^{\nu}(t)\rangle=\int_0^s\frac{E_{\nu,\nu}(-a[s-u]^{\nu})E_{\nu,\nu}(-a[t-u]^{\nu})}{(s-u)^{1-\nu}(t-u)^{1-\nu}}du$$
$$=\sum_{j,k=0}^{\infty}\frac{(-a)^{j+k}}{\Gamma(\nu j+\nu)\Gamma(\nu k+\nu)}\times\int_0^s(s-u)^{\nu(j+1)-1}(t-u)^{\nu(k+1)-1}du$$
$$=\sum_{j,k=1}^{\infty}\frac{(-a)^{j+k-2}}{\Gamma(\nu j)\Gamma(\nu k)}\times\int_0^s(s-u)^{\nu j-1}(t-u)^{\nu k-1}du$$
$$=\sum_{j,k=1}^{\infty}\frac{(-a)^{j+k}}{\Gamma(\nu j+1)\Gamma(\nu k)}s^{\nu j}t^{\nu k-1}\times{}_2F_1\left(1,1-\nu k,1+\nu j,\frac{s}{t}\right). \tag{B1}$$

X_{OU}^{ν} is nonstationary in contrast to the OU process. Thus it cannot be the fractional OU process we are looking for.

Furthermore, one can show that its variance does not lead to power-law behavior as required for anomalous diffusion. By using the property of the hypergeometric function [16] that ${}_2F_1(\alpha,\beta,\gamma,1)=\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)[\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)]^{-1}$, and the identity for gamma functions $x\Gamma(x)=\Gamma(1+x)$, one obtains the variance as

$$\langle[X_{\mathrm{OU}}^{\nu}(t)]^2\rangle=\sum_{j,k=1}^{\infty}(-a)^{j+k-2}t^{\nu j+\nu k-1}\times\frac{\Gamma(\nu j+\nu k-1)}{\Gamma(\nu j)\Gamma(\nu k)\Gamma(\nu j+\nu k)}$$
$$=\frac{1}{a^2t}\sum_{j,k=1}^{\infty}\frac{(-a)^{j+k}}{(\nu j+\nu k-1)\Gamma(\nu j)\Gamma(\nu k)}t^{\nu j+\nu k}$$
$$\leqslant\frac{1}{a^2t}\sum_{j=1}^{\infty}\frac{(-at^{\nu})^j}{\Gamma(\nu j)}\sum_{k=1}^{\infty}\frac{(-at^{\nu})^k}{\nu k\Gamma(\nu k)}, \tag{B2}$$

since $(\nu j+\nu k-1)\geqslant\nu k$ for $\nu\geqslant1$ and $j,k\geqslant1$. Thus

$$\langle[X_{\mathrm{OU}}^{\nu}(t)]^2\rangle\leqslant\frac{1}{at}\sum_{j=0}^{\infty}\frac{(-at^{\nu})^{j+1}}{\Gamma(\nu[j+1])}\sum_{k=1}^{\infty}\frac{(-at^{\nu})^k}{\Gamma(\nu k+1)}$$
$$=-t^{\nu-1}E_{\nu,\nu}(-at^{\nu})[E_{\nu,1}(-at^{\nu})-1]. \tag{B3}$$

For $at\to0$, one gets $E_{\nu,\nu}(at^{\nu})\sim1$ and $[E_{\nu,1}(-at^{\nu})-1]\sim-at^{\nu}$ such that

$$\langle[X_{OU}^{\nu}(t)]^2\rangle\lesssim t^{2\nu-1}. \tag{B4}$$

For large $t-\infty$, the Mittag-Leffler function has the following asymptotic series expansion [15]:

$$E_{\alpha,\beta}(z)=-\sum_{k=1}^{N}\frac{z^{-k}}{\Gamma(\beta-\alpha k)}+O(|z|^N), \tag{B5}$$

which is valid for $|\arg(-z)|<[1-(\alpha/2)]\pi$ and $z\to\infty$. It follows that

$$E_{\alpha,\alpha}(-t)\sim t^{-2}\qquad\text{for } t\to\infty, \tag{B6}$$

such that $E_{\nu,\nu}(-at^{\nu})\sim t^{-2\nu}$. On the other hand, $[E_{\nu,1}(-at^{\nu})-1]\sim-1$ as $+\to\infty$. Therefore, $\langle[X_{\mathrm{OU}}^{\nu}(t)]^2\rangle\leqslant t^{-\nu-1}$ as $t\to\infty$.

APPENDIX C

Let $C_*(s,t)$, $C_{\mathrm{RL}}(s,t)$, and $C_{\mathrm{W}}(s,t)$ be the correlation functions of SBM, RL-FBM, and standard FBM, respectively. Suppose these processes have zero means and they are appropriately normalized such that

$$C_*(t,t)=C_{\mathrm{RL}}(t,t)=C_{\mathrm{W}}(t,t). \tag{C1}$$

Then for $s,t\geqslant0$ and $1/2\leqslant H<1$,

$$C_*(s,t)\leqslant C_{\mathrm{RL}}(s,t)\leqslant C_{\mathrm{W}}(s,t). \tag{C2}$$

First note that for $s,t\geqslant0,s\leqslant t$,

$$C_*(s,t)=s^{2H}=2H\int_0^s(s-u)^{2H-1}du$$
$$\leqslant2H\int_0^s(s-u)^{H-1/2}(t-u)^{H-1/2}du$$
$$=C_{\mathrm{RL}}(s,t). \tag{C3}$$

$$C_W(s,t)=\frac{1}{2}[s^{2H}+t^{2H}-(t-s)^{2H}]$$
$$=H\int_0^s u^{2H-1}du+H\int_{t-s}^t u^{2H-1}du$$
$$=H\left\{\int_0^s\{(v^{H-1/2})^2+[(t-s+v)^{H-1/2}]^2\}dv\right\}$$
$$\geqslant2H\int_0^s v^{H-1/2}(t-s+v)^{H-1/2}dv=C_{\mathrm{RL}}(s,t). \tag{C4}$$

Combining Eqs. (C3) and (C4) gives Eq. (C2).

For $0<H\leqslant 1/2$, the inequality (C3) is reversed, whereas inequality (C4) remains valid. Since for $0<H<1$, $s<t$,

$$s^{H}\geqslant t^{H}-(t-s)^{H} \tag{C5}$$

then

$$2s^{H}\geqslant s^{H}+t^{H}-(t-s)^{H}, \tag{C6}$$

which implies

$$C_{*}(s,t)\geqslant C_{\mathrm{W}}(s,t). \tag{C7}$$

Hence

$$C_{\mathrm{RL}}(s,t)\leqslant C_{\mathrm{W}}(s,t)\leqslant C_{*}(s,t) \tag{C8}$$

for $0<H\leqslant 1/2$.

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